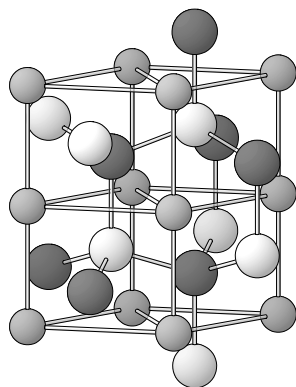


LiGaGe [2]; LiZnSb [3]

Structural features: 3D-framework of fused Li_6 trigonal prisms centered alternatively by Ga and Ge (displaced from the prisms centers). GaLi_6 trigonal prisms share edges to form a 3D-framework (the same is true for the GeLi_6 prisms). Ga and Ge form a tetrahedral 3D-framework. Substitution derivative of CaIn_2 . See Fig. IV.18.

Fig. IV.18. **LiGaGe**

Arrangement of Li_6 trigonal prisms (Li atoms small) and tetrahedral framework formed by Ga (dark) and Ge (light) atoms.

Bockelmann W., Schuster H.U. (1974) [1]

GaGeLi

$a = 0.4176$, $c = 0.6782$ nm, $c/a = 1.624$, $V = 0.1024$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.303		fourcapped trigonal prism Ga_4Li_6
Ga2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.688		fourcapped trigonal prism Ge_4Li_6
Li3	$2a$	$3m.$	0	0	0.0		rhombic dodecahedron $\text{Ga}_6\text{Ge}_6\text{Li}_2$

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.753

Experimental: single crystal, photographs, X-rays, $R = 0.097$

Remarks: Space group (194) $P6_3/mmc$ was tested and rejected ($R = 0.118$).

References: [1] Bockelmann W., Schuster H.U. (1974), Z. Anorg. Allg. Chem. 410, 233-240. [2] Bockelmann W., Jacobs H., Schuster H.U. (1970), Z. Naturforsch. B 25, 1305-1306. [3] Schroeder G., Schuster H.U. (1975), Z. Naturforsch. B 30, 978-979.